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Ordering and frustrations in generalized Ising chain

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Ordering and frustrations in generalized Ising chain

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Abstract. The Ising model on a one-dimensional monoatomic equidistant lattice with different nearest-neighbour and second-neighbour exchange interactions is researched. Generalized Kramers-Wannier transfer-matrix with translation on two periods of a lattice is introduced. A property similar to supercooling and superheating is detected. At the triple points phases are not individualized, but completely frustrated which corresponds to the phenomenon of critical opalescence. Exact analytical expressions for free energy, heat capacity and entropy including zero-temperature entropy are obtained. Various new special cases were analyzed and compared with all known results. All frustration fields for magnetization, frustration values for the zero-temperature entropy and magnetization are found.

1. Introduction

The first and most significant milestone in the theory of magnetism is Ernest Ising's publication of his work in 1925 [1], in which he presented an exact analytical solution of the problem of the magnetic moments of atoms (spins) located at the sites of a one-dimensional lattice connected by a short-range exchange interaction and an external magnetic field. In fact, in this work, the first theoretical magnetization curve was obtained, both for a ferromagnet and an antiferromagnet. And although the main desired result — a temperature phase transition from a disordered (paramagnetic) phase to an ordered magnetic state — was not obtained, this work and the model, later called the Ising model, attracted close and inexhaustible attention of researchers. At present, the Ising model, which long gone beyond the bounds of magnetism, has thousands and thousands of articles, reviews, monographs, conference proceedings, and their number is constantly growing.

The second significant stage in the theory of magnetism was the invention of a very effective method of the so-called transfer-matrix by Kramers and Wannier [2]. The essence of this method is that the calculation of the partition function of a giant number (2^N) of magnetic configurations is reduced to finding one principal (maximum) eigenvalue of a rather simple matrix. As a result, the Gibbs free energy and all the thermodynamic and magnetic characteristics of the system are expressed through this eigenvalue by simple differentiation with respect to temperature and magnetic field.

It was this invention that later allowed Onsager [3] to obtain an outstanding result — a phase transition in the Ising model on a two-dimensional square lattice, which laid the foundation for the rapid development of research in the physics of critical phenomena. In addition, the Onsager’s solution led to the appearance of exact solutions on other two-dimensional lattices: the triangular Ising net (Wannier [4]), the hexagonal lattice (Houtappel [5]), and the kagome Ising net (Kano and Naya [6]).

However, in spite of the complexity of all the previously considered generalizations, it is worth noting that so far the Kramers-Wannier transfer-matrix has been preserved when transferring only one translation of the lattice.

In this paper, the purpose was to generalize the Kramers-Wannier matrix method, which would set the transfer to two lattice translations, as well as to study of magnetic and thermodynamic properties of this model.

The results obtained in the study of the generalized Ising model can be used as prototypes for the study of quasi-one-dimensional polymeric and organic compounds [7, 8, 9].

2. Generalized Kramers-Wannier transfer-matrix

The generalized Ising model on a one-dimensional lattice with different nearest-and second-neighbour exchange interactions in external magnetic field is described by the Hamiltonian:

$$\mathcal{H}(s) = -J_1 \sum_{i=1,3,5,...}^{N-1} s_i s_{i+1} - J_2 \sum_{j=2,4,6,...}^{N} s_j s_{j+1} - \\ - J_1' \sum_{i=1,3,5,...}^{N-1} s_i s_{i+2} - J_2' \sum_{j=2,4,6,...}^{N} s_j s_{j+2} - H \sum_{i=1}^{N} s_i, \quad (1)$$

where J_1, J_2 are nearest-neighbour interactions, J_1', J_2' are second-neighbour interactions, H is an external magnetic field, N is the number of spins in the lattice, $s_i = \pm 1$.

Figure 1 illustrates a one-dimensional lattice of spins corresponding to the proposed generalized Ising model described by the Hamiltonian (1).

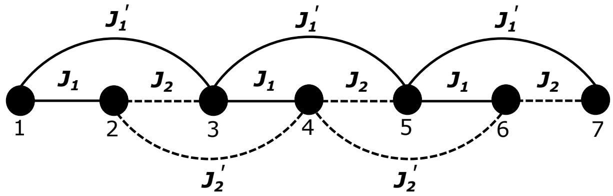


Figure 1. Nearest- and second-neighbours exchange interactions on one-dimensional lattice in generalized Ising model

In the considering method transfer-matrix of Kramers-Wannier all thermodynamic and magnetic quantities of the model are expressed only through its maximum eigenvalue λ_{max}. In consideration of the fact that in the Hamiltonian each sum runs over only half of sites, and not all spins of the lattice, the partition function in the thermodynamic limit ($N \to \infty$) takes the form:

$$Z_N = \lambda_{\max}^{N/2}. \quad (2)$$

Taking into account formulas for free energy, entropy, heat capacity and magnetization may be written in the following form:

$$F(H, T) = -\frac{T}{2} \ln \lambda_{\max}, \quad (3)$$

$$S(H,T) = \frac{1}{2}\ln\lambda_{\max} + \frac{T}{2\lambda_{\max}}\frac{\partial\lambda_{\max}}{\partial T}, \tag{4}$$

$$C(H,T) = \frac{T}{\lambda_{\max}}\frac{\partial\lambda_{\max}}{\partial T} + \frac{T^2}{2}\frac{\partial}{\partial T}\frac{1}{\lambda_{\max}}\frac{\partial\lambda_{\max}}{\partial T}, \tag{5}$$

$$M(H,T) = \frac{T}{2\lambda_{\max}}\frac{\partial\lambda_{\max}}{\partial H}. \tag{6}$$

Maximum eigenvalue of generalized Kramers-Wannier transfer-matrix may be found from the following expression:

$$\lambda_{\max} = \frac{\sqrt{a^2-4b+4y}-a}{4} + \sqrt{\left(\frac{\sqrt{a^2-4b+4y}-a}{4}\right)^2 - \frac{y}{2} - \frac{2c-ya}{2\sqrt{a^2-4b+4y}}}, \tag{7}$$

where

$$\begin{aligned}
&Q = \frac{p^3}{27}+\frac{q^2}{4}, \quad p = -\frac{b^2}{3}+ac-4d,\\
&q = -\frac{2b^3}{27}+\frac{bac}{3}+\frac{8bd}{3}-a^2d-c^2, \quad y = \sqrt[3]{\sqrt{Q}-\frac{q}{2}}+\sqrt[3]{-\sqrt{Q}-\frac{q}{2}}+\frac{b}{3},\\
&a = -2\left(\cosh\left[\frac{2H}{T}\right]e^{\left(J_1+J_1^{'}+J_2+J_2^{'}\right)/T}+e^{\left(-J_1+J_1^{'}-J_2+J_2^{'}\right)/T}\right),\\
&b = 2\left(2\cosh\left[\frac{2H}{T}\right]\left(e^{2\left(J_1^{'}+J_2^{'}\right)/T}-\cosh\left[2\left(J_1^{'}-J_2^{'}\right)/T\right]\right)+\right.\\
&\quad\left.+\left(e^{2J_1/T}\sinh\left[2\left(J_1^{'}+J_2+J_2^{'}\right)/T\right]+\,e^{-2J_1/T}\sinh\left[2\left(J_1^{'}-J_2+J_2^{'}\right)/T\right]\right)\right),\\
&c = -2e^{-\left(J_1+J_1^{'}+J_2+J_2^{'}\right)/T}\left(\cosh\left[\frac{2H}{T}\right]+e^{2(J_1+J_2)/T}\right)\left(e^{4J_1^{'}/T}-1\right)\left(e^{4J_2^{'}/T}-1\right),\\
&d = 16\sinh^2\left[\frac{2J_1^{'}}{T}\right]\sinh^2\left[\frac{2J_2^{'}}{T}\right].
\end{aligned}$$

3. Ordering in generalized Ising model

A detailed analysis of a large variety of possible variants of numerical values and signs of four exchange interaction parameters $J_1, J_1^{'}, J_2, J_2^{'}$ leads to the conclusion that only seven types of ordering (magnetic structures) may be realized in the ground state. The ferromagnetic structure corresponding to the conservation of the period of lattice translations, the internal energy of which in the ground state is equal to $E_f = -(J_1+J_2+J_1^{'}+J_2^{'})/2 - H$. The structure with doubling the period of lattice translations with internal energy $E_{af} = (J_1+J_2-J_1^{'}-J_2^{'})/2$. Also four structures $aaff$, $faaf$, $ffaf$ and $fffa$ with quadrupling of the lattice translation period, the internal energies of which are equal to: $E_{aaff} = (J_1^{'}+J_2^{'}-J_1+J_2)/2$, $E_{faaf} = (J_1^{'}+J_2^{'}+J_1-J_2)/2$, $E_{ffaf} = (J_1^{'}-J_2^{'})/2 - H/2$, $E_{fffa} = -(J_1^{'}-J_2^{'})/2 - H/2$, respectively. And the structure with tripling of the lattice translation with energy: $E_{ffa} = (J_1+J_2+J_1^{'}+J_2^{'})/6 - H/3$.

Taking into account different variants of signs of exchange interactions between the nearest (J_1, J_2) and second neighbours ($J_1^{'}$, $J_2^{'}$) leads to the fact that the system have many different variants of competing interactions.

Consider the most interesting case of competing interactions if $J_1 < 0, J_1^{'} < 0, J_2 < 0, J_2^{'} < 0$. This case, depending on the exchange interactions, can have up to three frustrating fields. We introduce the interaction coefficients: $R_1 = |J_1^{'}/J_1|$ and $R_2 = |J_2^{'}/J_2|$. The coefficient R_1 is defined by the ratio of interactions on odd lattice sites, and R_2 on even sites.

By comparing the energies of the respective configurations, we determine the frustrating fields [10]:

$$H_{\text{fr1}} = \begin{cases} -J_1 + 2J_1^{'} - J_2 + 2J_2^{'}, & 0 \le R_1 + R_2 \le 1; \\ 2J_1 - J_1^{'} - J_2 - J_2^{'}, & R_1 + R_2 \ge 1 \text{ and } J_1 \le J_2; \\ -J_1 - J_1^{'} + 2J_2 - J_2^{'}, & R_1 + R_2 \ge 1 \text{ and } J_1 \ge J_2. \end{cases} \tag{8}$$

$$H_{\text{fr2}} = \begin{cases} -J_1 + 2J_1^{'} - J_2 - 4J_2^{'}, & R_1 \ge R_2; \\ -J_1 - 4J_1^{'} - J_2 + 2J_2^{'}, & R_1 \le R_2. \end{cases} \tag{9}$$

$$H_{\text{fr3}} = \begin{cases} -J_1 - 2J_1^{'} - J_2, & R_1 \ge R_2; \\ -J_1 - J_2 - 2J_2^{'}, & R_1 \le R_2. \end{cases} \tag{10}$$

Next, we find the values of zero-temperature entropy and zero-temperature magnetization in the obtained frustrating fields.

The first frustrating field at $R_1 + R_2 < 1$.

This field corresponds to the transition between the antiferromagnetic phase and the phase with a tripling of the translation period.

$$S_{\text{fr}} = \ln\left\{\frac{2}{\sqrt{3}}\cos\left[\frac{1}{3}\arccos\left(\frac{3\sqrt{3}}{2}\right)\right]\right\} \approx 0.2812 \tag{11}$$

$$M_{\text{fr}} = \frac{1}{3} - \frac{4}{3\sqrt{23}}\sinh\left[\frac{1}{3}\operatorname{arsinh}\left(\frac{\sqrt{23}}{2}\right)\right] \approx 0.17701 \tag{12}$$

The first frustrating field at $R_1 + R_2 > 1$ and $J_1 < J_2$ or at $R_1 + R_2 > 1$ and $J_1 > J_2$.

In this field, a transition occurs between the $aaff$ and ffa phases or between the $faaf$ and ffa phases, depending on the values of J_1 and J_2. It may happen that $J_1 = J_2$, then the configurations with the quadrupling of the translation period of $aaff$ and $faaf$ become equal, thus, the frustrating fields will also become identical. However, even with different magnitudes of interactions J_1 and J_2 the values of the zero-temperature entropy and the zero-temperature magnetizations of the two transitions will be similar.

$$S_{\text{fr}} = \frac{1}{2}\ln\left\{\frac{2}{\sqrt{3}}\cos\left[\frac{1}{3}\arccos\left(\frac{3\sqrt{3}}{2}\right)\right]\right\} \approx 0.1406 \tag{13}$$

$$M_{\text{fr}} = \frac{1}{3} - \frac{4}{3\sqrt{23}}\sinh\left[\frac{1}{3}\operatorname{arsinh}\left(\frac{\sqrt{23}}{2}\right)\right] \approx 0.17701 \tag{14}$$

The value of zero-temperature entropy decreased by two times compared with the first frustrating field at $R_1 + R_2 < 1$, but the zero-temperature magnetization remained the same.

The first frustrating field at $R_1 + R_2 > 1$ and $J_1 = J_2$.

This is the ultimate case in which the $aaff$ and $faaf$ configurations become the same.

$$S_{\text{fr}} = \ln\left[\frac{1}{2}\left(\xi + \sqrt{\frac{2}{\xi} - \xi^2}\right)\right] \approx 0.1995, \tag{15}$$

where

$$\xi = \sqrt{\frac{4}{\sqrt{3}}\sinh\left[\frac{1}{3}\operatorname{arsinh}\left(\frac{3\sqrt{3}}{16}\right)\right]}.$$

$$M_{\text{fr}} = \sqrt{\frac{1}{283}\left(\frac{2}{f}+9\right) - f^2} - f \approx 0.1593, \tag{16}$$

where

$$f = \sqrt{\frac{3}{283}\left(1+\frac{16}{3\sqrt{3}}\sinh\left[\frac{1}{3}\operatorname{arsinh}\left(\frac{3\sqrt{3}}{16}\right)\right]\right)}.$$

The first frustrating field at $R_1 + R_2 = 1$.

Under this condition, the system degenerates into the usual (not generalized) Ising model with interactions between the nearest and second neighbours. The frustrating field is zero, and the entropy is equal to the natural logarithm of the golden ratio.

$$S_{\text{fr}} = \ln\left(\frac{1+\sqrt{5}}{2}\right) \approx 0.4812 \tag{17}$$

The second frustrating field at $R_1 > R_2$ or at $R_1 < R_2$.

When studying transitions from phases with tripling to phases with a quadrupling of the period of lattice translations with magnetization 1/2, it is important to know the values R_1 and R_2, it depends on where the system goes with increasing magnetic field. In particular, if $R_1 > R_2$, then the system undergoes a transition to the $ffaf$ configuration, and if $R_1 < R_2$, then the system switches to the $fffa$ configuration. However, the zero-temperature entropy and magnetization values for these two transitions do not differ.

$$S_{\text{fr}} = \frac{1}{2}\ln\left\{\frac{2}{\sqrt{3}}\cos\left[\frac{1}{3}\arccos\left(\frac{3\sqrt{3}}{2}\right)\right]\right\} \approx 0.1406 \tag{18}$$

$$M_{\text{fr}} = \frac{1}{3} + \frac{2}{3\sqrt{23}}\sinh\left[\frac{1}{3}\operatorname{arsinh}\left(\frac{\sqrt{23}}{2}\right)\right] \approx 0.4115 \tag{19}$$

The second frustrating field at $R_1 = R_2$.

If the interaction coefficients R_1 and R_2 are equal, we again arrive at the limiting case – we obtain the usual (not generalized) Ising model with interactions between the nearest and second neighbours in a magnetic field. There is a transition from the configuration with the tripling of the translation period directly into the ferromagnetic configuration, this may be written as $H_{\text{fr}2} = H_{\text{fr}3}$. Energies of quadruplicated configurations the $ffaf$ and $fffa$ are equal, so a plateau with a magnetization of 1/2 is not formed, and the system from the value 1/3 goes into a fully magnetized state.

$$S_{\text{fr}} = \ln\left\{\frac{1}{3}+\frac{2}{3}\cos\left[\frac{1}{3}\arccos\left(\frac{29}{2}\right)\right]\right\} \approx 0.3822 \tag{20}$$

$$M_{\text{fr}} = \frac{1}{3} + \frac{4}{3\sqrt{31}}\cos\left[\frac{1}{3}\arccos\left(\frac{\sqrt{31}}{2}\right)\right] \approx 0.6115 \tag{21}$$

The third frustrating field at $R_1 < R_2$ or at $R_1 > R_2$.

In this case, the zero-temperature entropy and magnetization values are written by the following expressions:

$$S_{\text{fr}} = \frac{1}{2}\ln\left(\frac{1+\sqrt{5}}{2}\right) \approx 0.2406 \tag{22}$$

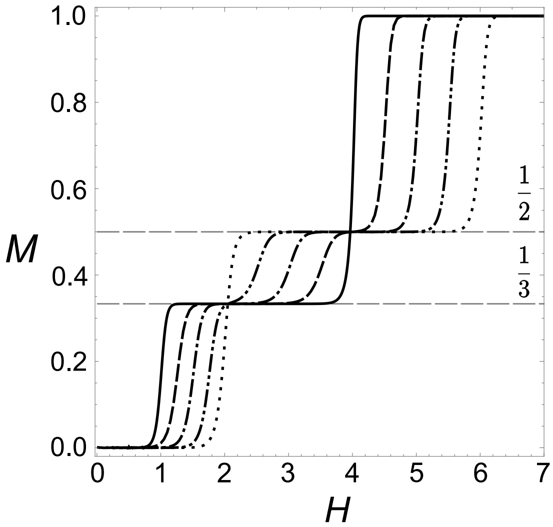


Figure 2. Magnetization of generalized Ising model for $J_1 < 0, J_1^{'} < 0, J_2 < 0, J_2^{'} < 0$; at $|R_1 - R_2| = 0$ (solid line), 0.25 (dashed line), 0.5 (dot-dashed line), 0.75 (dot-dot-dashed line), 1 (dotted line).

$$M_{\mathrm{fr}} = \frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right) \approx 0.7236 \tag{23}$$

The consideration of such a unique case is not over yet. A detailed analysis showed that a transition is possible from states with zero magnetization (af, $aaff$ or $faaf$) directly to the $ffaf$ or $fffa$ phase, bypassing the phase with tripling of the translation period (ffa). To do this, the following condition must be met: $|R_1 - R_2| \geq 1$, if $R_1 \geq R_2$, then a transition to the state $ffaf$ takes place, if vice versa $R_1 \leq R_2$, then to configuration $fffa$. The system will switch to the configuration with a tripling of the translation period, and then into the configuration with a quadrupling of the translation period, only if the condition is met: $0 \leq |R_1 - R_2| \leq 1$. This behaviour of magnetization is reflected in figure 2.

Putting $|R_1 - R_2| = 1$, which is equivalent to $H_{\mathrm{fr1}} = H_{\mathrm{fr2}}$, we get:

$$S_{\mathrm{fr}} = \frac{1}{2}\ln\left\{\frac{1}{3} + \frac{2\sqrt{7}}{3}\cos\left[\frac{1}{3}\arccos\left(-\frac{1}{2\sqrt{7}}\right)\right]\right\} \approx 0.2944 \tag{24}$$

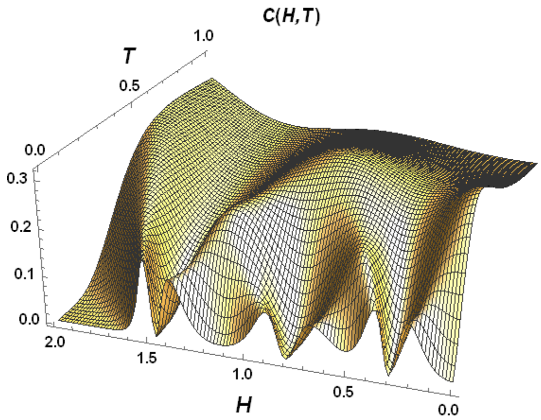
$$M_{\mathrm{fr}} = \frac{2}{\sqrt{21}}\cos\left[\frac{1}{3}\arccos\left(-\frac{3}{2}\sqrt{\frac{3}{7}}\right)\right] \approx 0.2417 \tag{25}$$

Given the various interactions defined on odd sites ($J_1, J_1^{'}$) and even sites ($J_2, J_2^{'}$), in a generalized Ising model there is an additional intermediate plateau with a magnetization of 1/2, in contrast to the usual (not generalized) Ising model.

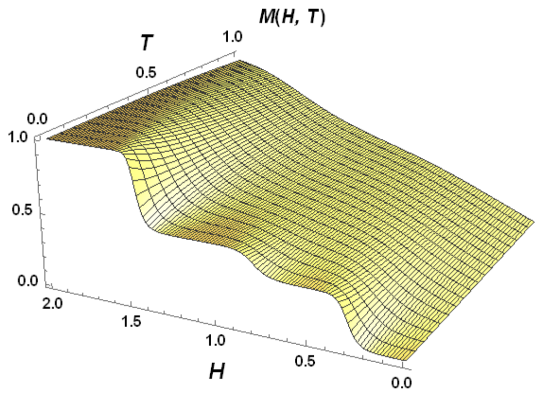
Figure 3a illustrates a three-dimensional graph of heat capacity as a function of temperature and magnetic field for the variant of competing interactions at $J_1 = -1, J_1^{'} = -0.7, J_2 = -1, J_2^{'} = -1.2$. The values of the magnetic field, where the heat capacity vanishes (for $T \to 0$), correspond to the values of the frustrating fields. In these fields, the magnetization is experiencing a saltus, as can be seen in figure 3b.

At equalities $J_1 = J_2$ and $J_1^{'} = J_2^{'}$ the intermediate plateau with magnetization 1/2 disappears, heat capacity and magnetization will be reduced to the variant of antiferromagnetic interactions between the nearest neighbours, considered in the usual (not generalized) Ising model [11, 12].

Studying the behaviour of the system at and near the points of frustration surprising results were obtained.



(a)



(b)

Figure 3. Heat capacity (a) and magnetization (b) as functions of temperature and magnetic field in generalized Ising model on linear chain at $J_1 = -1, J_1^{'} = -0.7, J_2 = -1, J_2^{'} = -1.2$.

In our case, as in thermodynamics, there was obtained a phenomenon when one phase exists in the region of another phase, and vice versa, the second phase exists in the region of the first phase. This situation is shown in figure 4. This phenomenon is in accordance with the phenomenon of supercooling and superheating.

In addition, at the points of convergence of several phases at once, the phases are not individualized, but significantly frustrated, since, in addition to converging phases, there are an infinite number of configurations without any translational invariance at these points, as evidenced by nonzero zero-temperature entropy. This phenomenon is quite similar to the phenomenon of critical opalescence. Smoluchowski [13] was the first who presciently predicted that the phenomenon of critical opalescence was due to the appearance of an infinite number of thermodynamic fluctuations at a triple point. It should be said that in modern language, in fact, at the triple point, the phenomenon of strong frustration occurs.

4. Conclusions

In this work the main results of the study of the magnetic and thermodynamic properties of the generalized Ising model, taking into account the interactions between the nearest and second

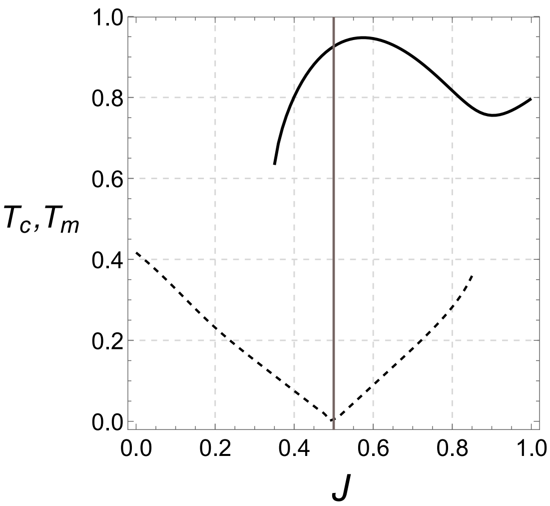


Figure 4. The position of the maximums of heat capacity in close proximity to frustration; T_c – temperature of the first maximum, T_m – temperature of the second maximum.

neighbours, different signs of exchange interactions, and an external magnetic field are presented. An exact analytical solution for the generalized Ising model in a magnetic field is obtained. The sequence of exact expressions for zero-temperature entropies and magnetizations is derived. A qualitative coincidence with the phenomenon of critical opalescence in frustration points and supecooling and superheating in close proximity to frustration is observed.

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